

DEVELOPMENT OF PCA-BASED FAULT DETECTION SYSTEM BASED ON
VARIOUS MODES OF NOC MODELS FOR CONTINUOUS-BASED PROCESS

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ABSTRACT

Multivariate statistical techniques are used to develop detection methodology for abnormal process behavior and diagnosis of disturbance which causing poor process performance (Raich and Cinar, 2004). Hence, this study is about the development of principal component analysis (PCA) -based fault detection system based on various modes of normal operating condition (NOC) models for continuous-based process. Detecting out-of-control status and diagnosing disturbances leading to the abnormal process operation early are crucial in minimizing product quality variations (Raich and Cinar,2004). The scope of the proposed study is to run traditionally multivariate statistical process monitoring (MSPM) by defining mode difference in variance for continuous-based process. The methodology use to identify and detection of fault which undergo two phase which phase I is off-line monitoring while phase II is on-line monitoring. As a result, it will be analyze and compared of the implementing traditional PCA of Single NOC modes and Multiple NOC modes. Particularly, this study is critically concerned more on the performance during the fault detection operations comprising both off-line and on-line applications, hence it will analyze until fault detection and comparing between two modes of NOC data.

ABSTRAK

Multivariat teknik statistik yang digunakan untuk membangunkan kaedah pengesanan proses untuk tingkah laku yang tidak normal dan diagnosis gangguan yang menyebabkan prestasi proses miskin (Raich dan Cinar, 2004). Oleh itu, kajian ini adalah mengenai pembangunan analisis komponen utama (PCA) berasaskan kesalahan sistem pengesanan berdasarkan pelbagai mod keadaan operasi normal (NOC) model untuk proses yang berterusan berasaskan. Mengesan status out-of-kawalan dan mendiagnosis gangguan yang membawa kepada operasi proses abnormal awal adalah penting dalam mengurangkan variasi kualiti produk (Raich dan Cinar, 2004). Skop kajian yang dicadangkan adalah untuk menjalankan pemantauan tradisional multivariat proses berstatistik (MSPM) dengan menentukan perbezaan mod dalam varians proses yang berterusan berasaskan. Metodologi yang digunakan untuk mengenal pasti dan pengesanan kesalahan yang menjalani dua fasa fasa yang saya off-line pemantauan manakala fasa II adalah on-line pemantauan. Hasilnya, ia akan menganalisis dan berbanding PCA pelaksana tradisional mod Single NOC dan Pelbagai mod NOC. Terutama sekali, kajian ini secara kritikal berkenaan lanjut mengenai prestasi semasa operasi pengesanan kesalahan yang terdiri daripada kedua-dua aplikasi off-line dan on-line, maka ia akan menganalisis sehingga pengesanan kerosakan dan membandingkan antara dua mod data NOC.

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CHAPTER 1

INTRODUCTION

1.1 Background of Proposed Study

Statistical process control (SPC) is the basic performance of monitor and detection of abnormal process (Zhao et al., 2004). According to MacGregor and Kourti (1995) the main objective of SPC is to monitor the process performance over time in order to verify the status of the process whether it is remaining in a “state of statistical control” or not. However, most SPC methods are based on charting only a small number of variables and examining them one at time (MacGregor and Kourti, 1995). As a result, multivariate statistical process control (MSPC) has been proposed especially to monitor multivariable process (Kumar and Madhusree, 2001; Kano et al., 2002; Zhao et al., 2004; MacGregor et al., 1995; Maestri et al. 1995). According to Kourti et al. 1995, multivariate method can treat and extract information simultaneously on the directionality of the process variation. Jackson and Mudholkar (1979) investigated principal component analysis (PCA) as a tool of MSPC and introduce a residual analysis. Typically, the Shewhart-type control chart is applied,

for depicting the progression of two different types of monitoring statistics, namely as T^2 and Q statistic. The T^2 statistics is a measure of the variation within PCA model while Q statistic is a measure of the amount of variation not captured by the PCA modes. When PC's is being scaled by the reciprocal of its variance, it will compute same role as T^2 irrespective of the amount of variance it's explain in the Y matrix, which Y is matrix of mean centered and scaled measurements. T^2 is not sufficient for first PC because it only detect whether the variation in the quality variables in the plane or not. Kresta et al., (1991) say new event can be detected by computing the squared prediction error (SPE) or also known as Q statistics. According to Jackson, (1991) and Nomikos and MacGregor (1995) Q statistics represents the square perpendicular distance of a new multivariate observation from the plane. Q statistics also represent unstructured fluctuation that cannot be accounted for by the model when the process is "in control". Hence it will be more effective multivariate control chart when T^2 chart on dominant orthogonal PC's plus a SPE chart.

1.2 Problem Statement

In order to ensure the successfulness of any operation, it is important to detect process upsets, equipment malfunctions or other special events as early as possible and then to diagnose and remove the factors that cause those events. However, Zhao et al., (2004) mentioned that a process which is having multiple operating modes tends trigger continuous warning signal even when the process itself is operating under another steady-state. In other word, the comprehensive mode is too sensitive as

it will show the false alarm although the process are normal. Hence, MSPC is the only method, of which, the data is treated simultaneously into a single monitoring by way of reducing the dimensionality of the data observed without losing any of important information.

1.3 Research Objectives

The main purpose of this research is to study the impact of applying various modes of normal operating condition (NOC) in terms of the number of samples and variable variations on the process monitoring performance for continuous-based process. Therefore, the main objectives of this research are:

- i. To develop the conventional MSPM method based on a single NOC
- ii. To implement the conventional MSPM method based on different modes of NOC.
- iii. To analyze the monitoring performance between system (i) and (ii).

1.4 Research Question

- i. What is the main impact of reducing the number of samples as well as variations on the monitoring performance?
- ii. What are the criteria should be used in selecting the NOC model?

1.5 Scopes of Study

Scope of propose study are on the development of PCA-based fault detection system based on various modes of NOC models for continuous-based process. There are three main scope will be investigated using MATLAB.

- i. The conventional MSPM method will be develop based on single NOC mode. The linear PCA algorithm is used for reducing the multivariate data dimensions.
- ii. The MSPM will be run traditionally by implementing different mode, which in this research is on two modes. According to Zhao et al. (2004),in spite of the success of applying PCA based MSPM tools to process data for detecting abnormal situations, when these tools are applied to a process with multiple operating modes, many missing and false alarms appear even when the process itself under other steady-state nominal operating conditions.
- iii. As all data have been obtained, it will be analyze further with two multivariate control charts namely Hotelling's T^2 and Squared Prediction Errors (SPE) statistic for the fault detection operation.

1.6 Contributions

- i. A new set of criteria is proposed for selecting the optimized NOC data for monitoring.
- ii. As a result of (i), the monitoring performance can be enhanced in terms of missing and false alarm.

1.7 Organization of This Report

The new monitoring algorithm has been proposed in this study by developing PCA-based fault detection system based on various modes of NOC models for continuous-based process. Hence, this report is divided into five main chapters. The first chapter discusses the background of the works which includes the problem statement, objectives, scopes and contributions. **Chapter II** which is literature review describes the fundamental of MSPC and justification of applying PCA in MSPM frameworks. **Chapter III** explains the research methodology of this study. **Chapter IV** presents some of the preliminary results. Conclusions and further research works are given in **Chapter V**.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

According to Venkatasubramaniam, Rengaswamy, Kavuri and Yin (2003) MSPM tools are data driven technique that generally reduce the dimension of process data and extract key features and trends that are of interest to plant personnel. MSPM tools used to reduces dimensions of process data, like PCA and subsequent refinements, which have show great success. In chapter 2, we will discuss on the fundamental or theory of process monitoring on MSPM using PCA tools, process monitoring issues and extension and justification of applying PCA in MSPM frameworks. Lastly, a summary is given at the end of this chapter.

2.2 Fundamentals / Theory of Process Monitoring on MSPM Using PCA Tools

Reformation and upgrading of conventional Statistical Process Control (SPC) method has produce MSPC. MSPC tools such as principal component analysis (PCA) were used to reduce the explaining dimension of the process data. Maestri et al. say this method has show great success and particularly suited to data set comprising correlated and collinear variables. Ge and Song (2008) define process data as different group based, for instance, on variation in the operating capacity, seasonal variations or changes in the feedstock characteristics and also on modifications in the operation strategies. From a geometric point of view, whenever such as a change occurs, the process data tend to group into a new cluster in a different location in the high dimensional space containing the process normal operating region. However when the data is considered belong to a unique normal operating region, the volume of this region becomes incorrectly large. Zhao et al, (2006) say this region will lead to an increasing number of missing and false alarm. According to Zhao et al, (2004) when PCA based MSPC tools applied to a process with multiple operating modes, many missing and false alarm can appear even when the process itself is operating under other steady-state nominal operating conditions. Particularly this technique is for reducing the number of dimensions used from the original data as well as projected them into a number of uncorrelated variables, by means of forming the appropriate linear combinations of the original variables. Hence, MSPC is the only method where the data is treated simultaneously by way of reducing the dimensionality of the data observed without losing any of important information. In addition, this method can reduce the burden of constructing a large amount of single-variable control charts and enable detecting events that are

impossible or difficult to detect from the single-variable control charts (Phatak, 1999).

According to Venkatasubramaniam et al, (2003) multivariate statistical techniques are powerful tool that capable to compressing data and reducing its dimensionality. Hence the essential information is retained and easy to analyze than the original huge data set. Moreover, it is able to handle noise and correlation to extract true information effectively. Initially, PCA method is proposed by Pearson (1901) later, it been develop by Hotelling (1947). This is a standard multivariate technique which has been including in many textbooks (Jackson, 1991; Anderson, 1984) and research paper (Wold, Esbensen and Geladi, 1987; Wold, 1978). Venkatasubramaniam et al, (2003) say PCA is based on orthogonal decomposition of the covariance matrix of the process variables along directions that explain the maximum variation of the data. Yu and Zhang say this method involved a mathematical procedure that transforms a number of correlated variables into a smaller number of uncorrelated variables, which are called principal component.

2.3 Extensions of Principal Component Analysis

There are many extension of Principle Component Analysis (PCA) which is some of these is Kernel of PCA, Multiway-PCA, , Three Modes PCA and many more.

2.3.1 Kernel of PCA

Some extension of PCA is nonlinear principle components (NLPCA) or also Kernel PCA (KPCA). According to Vidal, Ma, and Sastry, (2005) KPCA is method of identifying a nonlinear manifold from sample points. NLPCA is a standard solution based on embedding the first data into a higher space, then applying PCA. As a result it will give large dimension space, so the eigen value is being decomposition or also known as kernel matrix.

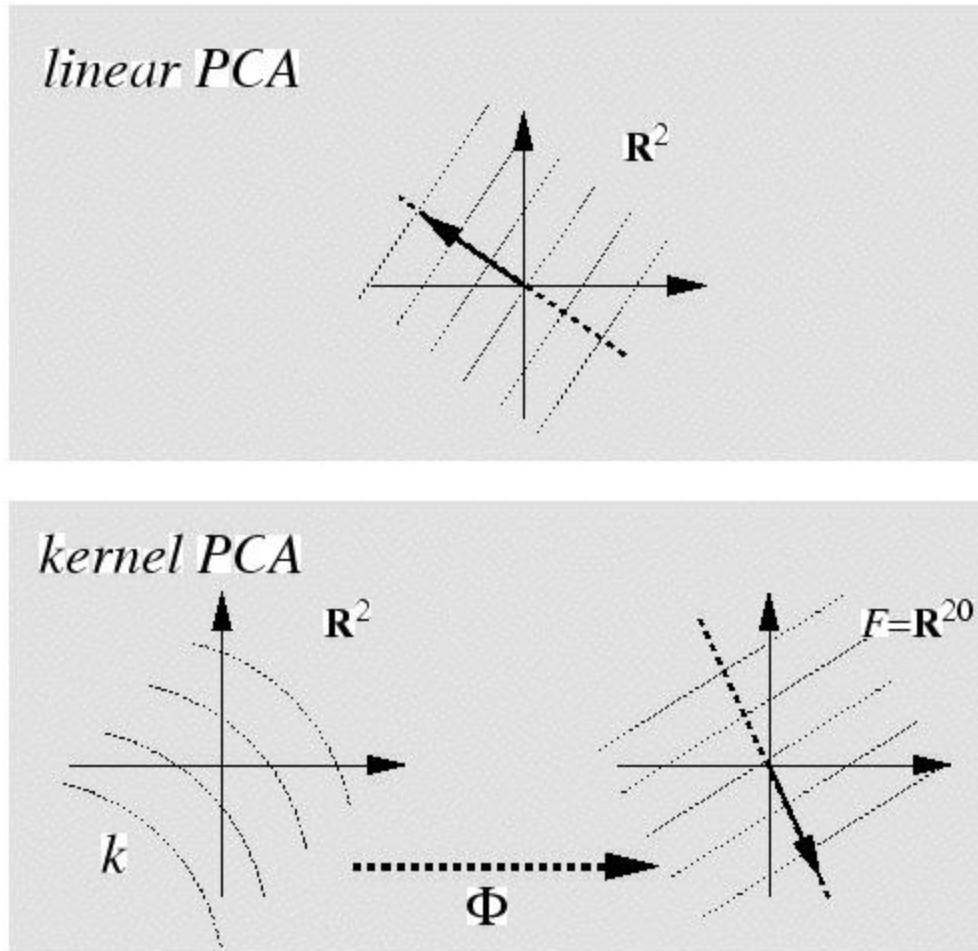


Figure 2.1 Linear PCA and Kernel PCA

From Figure 2.1 above, it shows the basic idea of kernel PCA. By using a nonlinear function k instead of the standard dot product, we implicitly perform PCA in a possibly high dimensional space F which is nonlinearly related to input space. The dotted lines are contour lines of constant feature value. Suppose that the number of observations m exceeds the input dimensionality n . In linear PCA, most samples are nonzero eigen values (Welling, nd). While for Kernel PCA variable will be nonzero eigen values. Thus, this is not necessarily a dimensionality reduction (Scholkopf, Smola and Muller, 2001). Furthermore, it may not be possible to find an exact preimage in input space of a reconstructed pattern based on a few of the eigenvectors. One of the disadvantages of KPCA is that, in practice, it is difficult to determine which kernel function to use because the choice of the kernel naturally depends on the nonlinear structure of the manifold to be identified (Vidal, Ma, and Sastry, 2005). In fact, learning kernels is an active topic of research in machine learning.

2.3.2 Multi-way-PCA

A monitoring approach using a multivariate statistical modelling technique namely multi-way principle component analysis is a method that overcomes the assumption that the system is at steady state and it provides a real time monitoring approach for continuous processes (Chen and McAvoy, 1998). Recently MacGregor and Nomikos (1992) and Nomikos and MacGregor (1994) employed multiway PCA (MPCA) to extend multivariate SPC methods to batch processes. This multi-way PCA model can detect fault in advance compared to other monitoring approaches as it will analyze a historical reference distribution of the measurement trajectories from

past successful batches (Nomikos and MacGregor, 1995). Besides Nomikos et al. also say that the latent-vector space is reducing as the variation in the trajectories is characterized.

This make multi-way PCA is a useful procedure because each dynamic response signature is highly auto-correlated. Gallagher, Wise and Stewart (1996) say the correlation at different times within each signature, hence there is a high degree of correlation between signatures. Wold et al.(1987) has discuss that multi-way PCA will allows the multivariate data to be described in far fewer components than original variables. The multi-way PCA procedure can be described as follows. The data from a historical database of batch runs are organized in a three-way array X ($I \times J \times K$). The batch runs (I) are organized along the vertical axis, the measurement variables (J) along the horizontal axis, and their time evolution (K) occupies the third dimension. Usually, the minimum duration of the batch process defines the time length of a batch (K) and the data are synchronized based on a trigger variable whose change indicates the beginning of the batch. Nomikos et al. (1996) say multi-way PCA will give a great result as more information related with analysis is provided such as quantities from mass or energy balances, properties related to quality, and degradation rates. Hence, X is decomposed into scores vectors t and loadings vectors p using traditional principal components analysis (PCA) (Jackson and Mudholkar, 1979, Wold, 1987).

The p -loading matrices, which define the reduced space upon the actual data are projected and summarize the time variation of the measurement variables around the average trajectories. The elements are the weights applied to the observations of a particular batch to give the t -scores for this batch which each element of a t -vector corresponds to a single batch and represent the projection of this batch onto the

reduced space. Finally, the sum of squared residuals for a given batch represents the squared distance of this batch perpendicular to the reduced space. A small number (R) of principal components usually 3 to 5 can express most of the variability in the batch data since the measurement variable are highly cross-correlated with one another and highly auto-correlated over time (Nomikos et al.,1996).

A process abnormality will result in poor quality product, hence multi-way PCA will help to detect and classify the cases. This is because multi-way PCA is an easily interpret tool which characterized batches based on their process operation. Then it is up to the engineers to remove the root cause and eliminate any future appearances of this fault. In some cases, MPCA might detect an abnormal behavior which may not have an immediate impact on quality, but may constitute an alarm for an incipient equipment failure such as an agitator or sensor deterioration. In these cases, one will have the opportunity to correct such process deteriorations which otherwise could lead to permanent malfunctions (Nomikos et al., 1996; Gallagher et al., 1996;Chen et al. 1998).

2.3.3 Three-Mode PCA

Tucker (1963) was first formulated the three-mode model principal component analysis or also known as Tucker3 model and it subsequently extended in articles by Tucker (1964, 1966) and Levin (1963). Kroonenberg and Leeuw say the articles review on the mathematical description and programming aspects of the model. In term of multidimensional scaling references to the mode 1 occur frequently (Harshman, 1970; Jennrich, 1972; Carroll & Chang, 1972; Takane , Young & de Leeuw, 1977), hence the Tucker3 mode 1 is the general mode 1

comprising various individual differences models. Tucker (1972), Carroll & Wish (1974), and Takane, Young & de Leeuw (1977) has discuss more on the relationships between multidimensional scaling and three-mode PCA. In article by Tucker (1966) remarks that the procedures "do not produce a least squares approximation to the data. Investigations of the mathematics of a least squares fit for three-mode factor analysis indicates a need for an involved series of successive approximations. "The procedures described in the sequel are designed to provide least squares estimates of the parameters in the three -mode model. The alternating least squares approach used can also be extended to accommodate other levels of measurement, as has been recently demonstrated by Sands & Young (1980) for a more restricted model.

Three-way data are data that can be classified in three ways. For an example is scores of a number of subjects on different variables measured on different occasions. Three-mode principal components analysis (Tucker, 1966) is a method for summarizing three-way data, and is a generalization of standard two-way principal components analysis (PCA). In two-way PCA the data are decomposed into two matrices, namely the component scores matrix and the component loading matrix. In three-mode PCA, the three-way data are decomposed into three component matrices, where the numbers of components to be used are not necessarily equal for each component matrix. When the numbers of components are not suggested by the nature of the data, a method is needed to indicate these numbers. In order to choose the numbers of components, Tucker (1966) proposed the application of a method ordinarily used in two-way PCA. However, it is not clear that this method is suitable for use in three-way problems. Therefore, a new method is proposed for indicating

the numbers of components in three-mode PCA, and this method is compared to two methods ordinarily used in two-way PCA by means of a simulation study.

Timmerman and Kiers (2000) three-mode PCA model is usually fitted to the data by Tuckals3 which is an alternating least squares algorithm. Unfortunately, this kind of algorithm may end in a local optimum. At the cost of computational effort, the possibility of missing the global optimum can be reduced by using multiple ‘starts’ for a single three-mode PCA model. Since the new method of determining the numbers of components requires a large number of three-mode PCAs, it is useful to examine the necessity of using multiple starts. In several applications of three-mode principal component analysis to sets of correlation matrices, results turned out to be very similar to results obtained via perfect congruence analysis for weights (Louwerse and Smilde, 2000). Three-mode PCA is meant for the analysis of possibly preprocessed three-way data x_{ijk} that give the score of individual i on variable j at measurement occasion k , $i=1,...,I$, $j=1,...,J$, $k=1,...,K$. In 3MPCA, as in PCA, matrices A and B are found that summarize the individuals and the variables, respectively, but in addition, a matrix C is found that summarizes the occasions. Usually, in three-mode PCA these matrices are all referred to by the general term “component matrices” and a distinction between component scores and loadings is not made (Kiers and Mechelen, 2001).